Lecture 1: Introduction to Data Assimilation

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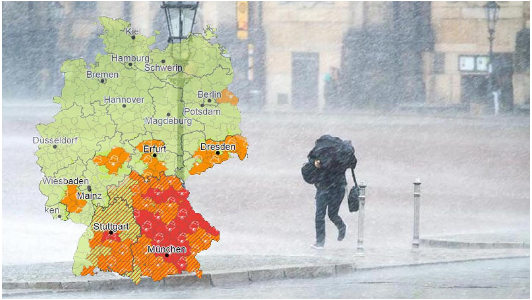
CEMRACS Data Assimilation and Reduced Modeling for High Dimensional Problems

Outline

What is Data Assimilation?

The seamless integration of large data sets into sophisticated computational models provides one of the central challenges for the mathematical sciences in the 21st century. When the computational model is based on dynamical systems, and the data set is time ordered, the process of combining models and data is called data assimilation.

Sebastian Reich and Andrew Stuart, SIAM News 2015



source: https://www.focus.de/panorama/videos/wettervorhersage-unwettergefahr-hier-drohen-starkregen-und-hagel_id_5763860.html

Applications of Data Assimilation

Data assimilation provides important techniques for the incorporation of data in models in various fields of science and engineering:

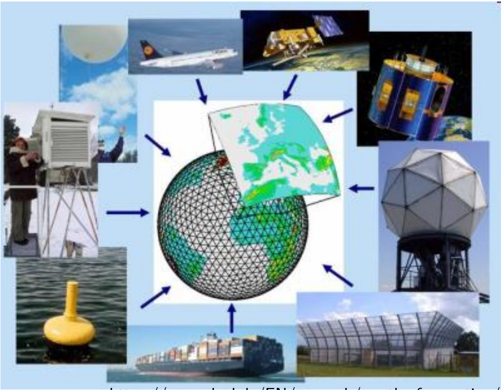
Numerical Weather Prediction

extrapolation of the present state of the atmosphere using computational models into the future

Oil reservoir modeling

Biological systems

Different observation systems



source: https://www.dwd.de/EN/research/weatherforecasting/num_modelling/02_data_assimilation/data_assimilation_node.html

Applications of Data Assimilation

Data assimilation provides important techniques for the incorporation of data in models in various fields of science and engineering:

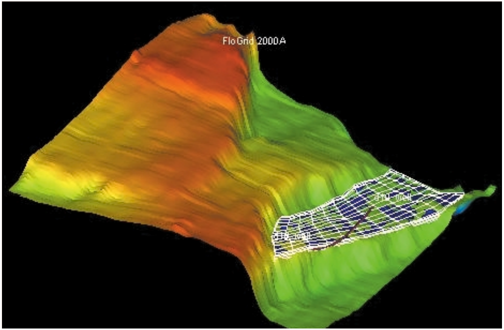
Numerical Weather Prediction

Oil reservoir modeling

improvement of the accuracy of the reservoir simulator by data

Biological systems

Reservoir in the Gulf of Mexico



source: Christie et al.

Applications of Data Assimilation

Data assimilation provides important techniques for the incorporation of data in models in various fields of science and engineering:

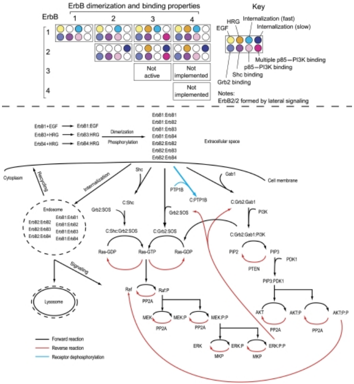
Numerical Weather Prediction

Oil reservoir modeling

Biological systems

confront biological models with measurement data

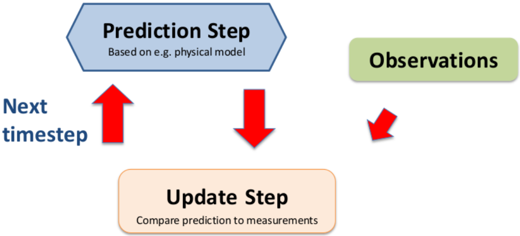
ErbB signaling pathways



source: Chen et al.

Challenges in Data Assimilation

- **High-dimensional problems.**
- **Highly nonlinear forward models.**
- **Robustness of data assimilation algorithms w.r.t. to numerical / model error.**
- **Assessment of uncertainty in the predictions.**



Mathematical Formulation of the Problem

We assume a model of the unknown z in the form of

$$\begin{aligned} z_{n+1} &= \Psi(z_n) + \zeta_n\,, \qquad n \in \mathbb{N} \\ z_0 &\sim \mathcal{N}(m_0, C_0) \end{aligned}$$

with $\Psi \in C(\mathbb{R}^{n_z}, \mathbb{R}^{n_z})$, $\zeta = (\zeta)_n$ an iid sequence with $\zeta_0 \sim \mathcal{N}(0, \Sigma)$, $\Sigma > 0$, z_0 and ζ are assumed to be independent.

There is a true trajectory of z that produces noisy observations

$$y_{n+1} = H z_{n+1} + \eta_{n+1}\,, \qquad n \in \mathbb{N}$$

with $H \in \mathcal{L}(\mathbb{R}^{n_z}, \mathbb{R}^{n_y})$ and $\eta = (\eta)_n$ an iid sequence, independent of (z_0, ζ) with $\eta_1 \sim \mathcal{N}(0, \Gamma)$, $\Gamma > 0$.

The aim of **data assimilation** is to characterize the conditional distribution of z_n given the observations.

Mathematical Formulation of the Problem

The discrete dynamics

$$z_{n+1} = \Psi(z_n) + \zeta_n\,, \qquad n \in \mathbb{N}\,, \quad z_0 \;\sim\; \mathcal{N}(m_0, C_0)$$

often result from the solution of an ordinary differential equation (ODE)

$$\frac{\mathrm{d}z}{\mathrm{d}t} = f(z)\,, \quad z(0) = z_0$$

for given right hand side (r.h.s.) $f \in C^1(\mathbb{R}^{n_z}, \mathbb{R}^{n_z})$.

In this case, Ψ is the solution operator for the ODE, i.e.

$$\begin{aligned} z(t) &= \Psi(z_0; t)\,, \quad t \in (0, \infty) \\ \Psi(z_0; t+s) &= \Psi(\Psi(z_0; s); t)\,, \quad s, t \in (0, \infty) \\ \Psi(z_0; 0) &= z_0\,. \end{aligned}$$

For some fixed $h > 0$, we define $\Psi(\cdot) = \Psi(\cdot; h)$ linking the discrete dynamics with continuous-time ODEs.

Mathematical Formulation of the Problem

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$$z_{n+1} = \Psi(z_n) + \zeta_n\,, \qquad n \in \mathbb{N}\,, \quad z_0 \ \sim \ \mathcal{N}(m_0, C_0)$$

with $\zeta = (\zeta)_n$ an iid sequence with density $\rho(\cdot)$, $z_0 \perp \zeta$.

Then, $(z_j)_n$ is a Markov chain with

$$\mathbb{P}(z_{j+1}|z_j) = \rho(z_{j+1} - \Psi(z_j))$$

and

$$\mathbb{P}(z_{j+1} \in A|z_j) = \int_A \rho(z_{j+1} - \Psi(z_j))\mathrm{d}z_{j+1}\,.$$

Mathematical Formulation of the Problem

The discrete dynamics

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The function $p : \mathbb{R}^{n_z} \times \mathcal{B}(\mathbb{R}^{n_z}) \to \mathbb{R}^+$ is a **Markov kernel** if

- for each $z \in \mathbb{R}^{n_z}$, $p(z, \cdot)$ is a probability measure on $(\mathbb{R}^{n_z}, \mathcal{B}(\mathbb{R}^{n_z}))$
- $z \mapsto p(z, A)$ is $\mathcal{B}(\mathbb{R}^{n_z})$-measurable for all $A \in \mathcal{B}(\mathbb{R}^{n_z})$.

Mathematical Formulation of the Problem

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and

$$\mathbb{P}(z_{j+1} \in A|z_j) = \int_A \rho(z_{j+1} - \Psi(z_j))\mathrm{d}z_{j+1}\,.$$

We define the Markov kernel

$$p(z, A) = \int_A \rho(x - \Psi(z))\mathrm{d}x$$

with pdf

$$p(z, x) = \rho(x - \Psi(z))$$

Mathematical Formulation of the Problem

If $z_j \sim \mu_j$ with pdf ρ_j, then

$$\begin{aligned}
\mu_{j+1}(A) &= \mathbb{P}(z_{j+1} \in A) \\
&= \int_{\mathbb{R}^{n_z}} \mathbb{P}(z_{j+1} \in A | z_j) \rho_j(z_j) \mathrm{d}z_j \\
&= \int_{\mathbb{R}^{n_z}} p(z, A) \rho_j(z) \mathrm{d}z
\end{aligned}$$

and

$$\begin{aligned}
\rho_{j+1}(x) &= \int_{\mathbb{R}^{n_z}} p(z, x) \rho_j(z) \mathrm{d}z \\
&= \int_{\mathbb{R}^{n_z}} \rho(x - \Psi(z)) \rho_j(z) \mathrm{d}z \,.
\end{aligned}$$

We define the map

$$\rho_{j+1} = \mathcal{P} \rho_j$$

with P being the operator

$$(\mathcal{P}\pi)(x) = \int_{\mathbb{R}^{n_z}} \rho(x - \Psi(z)) \pi(z) \mathrm{d}z \,.$$

Bayes's Formula as a Map

Bayes's formula states

$$\mathbb{P}(a|b) = \frac{1}{\mathbb{P}(b)}\mathbb{P}(b|a)\mathbb{P}(a)\,.$$

We can view the application of Bayes' theorem as a nonlinear map $\mathcal{L}$ from the prior $\mathbb{P}(a)$ to the posterior $\mathbb{P}(a|b)$ given by

$$\mathbb{P}(a|b) = \frac{\mathbb{P}(b|a)\mathbb{P}(a)}{\int_{\mathbb{R}^n}\mathbb{P}(b|a)\mathbb{P}(a)\mathrm{d}a} =: \mathcal{L}(\mathbb{P}(a))$$

Smoothing Problem

Find the signal z on a discrete time interval $\mathfrak{N}_0 = \{0, \ldots, N\}$

$$
\begin{aligned}
z_{n+1} &= \Psi(z_n) + \zeta_n \,, \qquad j \in \mathfrak{N}_0 \\
z_0 &\sim \mathcal{N}(m_0, C_0) \qquad \zeta_0 \sim \mathcal{N}(0, \Sigma)
\end{aligned}
$$

from given data y on the discrete time interval $\mathfrak{N} = \{1, \ldots, N\}$

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y_{n+1} = H z_{n+1} + \eta_{n+1} \,, \qquad j \in \mathfrak{N} \,, \qquad \eta_1 \sim \mathcal{N}(0, \Gamma) \,.
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$$y_{n+1} = H z_{n+1} + \eta_{n+1}\,, \qquad j \in \mathfrak{N}\,, \qquad \eta_1 \sim \mathcal{N}(0, \Gamma)\,.$$

- **Prior** μ_0

$$\mathbb{P}(z_0, \dots, z_N) = \prod_{n=0}^{N-1} \mathbb{P}(z_{n+1}|z_n)\mathbb{P}(z_0)$$

with

$$\mathbb{P}(z_0) \propto \exp(\frac{1}{2}|z_0 - m_0|^2_{C_0})$$

and

$$\mathbb{P}(z_{n+1}|z_n) \propto \exp(\frac{1}{2}|z_{n+1} - \Psi(z_n)|^2_{\Sigma})\,.$$

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- **Prior** μ_0

$$\mathbb{P}(z_0, \dots, z_N) \propto \exp(-\Theta(z_0, \dots, z_n))$$

with

$$\Theta(z_0, \dots, z_N) = \frac{1}{2}|z_0 - m_0|^2_{C_0} + \sum_{n=0}^{N-1} \frac{1}{2}|z_{n+1} - \Psi(z_n)|^2_{\Sigma}\,.$$

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- **Likelihood**

$$\mathbb{P}(y_1, \dots, y_N | z_0, \dots, z_N) = \prod_{n=0}^{N-1} \mathbb{P}(y_{n+1} | z_0, \dots, z_N)$$

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- **Likelihood**

$$\begin{aligned} \mathbb{P}(y_1, \dots, y_N | z_0, \dots, z_N) &= \prod_{n=0}^{N-1} \mathbb{P}(y_{n+1} | z_0, \dots, z_N) \\ &\propto \exp(-\Phi(z_0, \dots, z_n; y_1, \dots, y_n) \end{aligned}$$

with $\Phi(z_0, \dots, z_n; y_1, \dots, y_n) = \sum_{n=0}^{N-1} \frac{1}{2} |y_{n+1} - H z_{n+1}|_\Gamma^2$

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$$y_{n+1} = H z_{n+1} + \eta_{n+1}\,, \qquad j \in \mathfrak{N}\,, \qquad \eta_1 \sim \mathcal{N}(0, \Gamma)\,.$$

Bayes' Theorem

The posterior smoothing distribution on $z_0, \ldots, z_n | y_1, \ldots, y_n$ is given by

$$\mathbb{P}(z_0, \ldots, z_n | y_1, \ldots, y_n) \propto \exp(-\Phi(z_0, \ldots, z_n; y_1, \ldots, y_n) - \Theta(z_0, \ldots, z_n))\,.$$

Well-Posedness of the Smoothing Problem

Well-posedness

Let $Y = (y_1, \dots, y_N)$ and $Y' = (y'_1, \dots, y'_N)$ be both contained in a ball of radius R. We denote by μ and μ' the posterior distributions associated with the two data sets Y and Y'. Further, assume that $\tilde{z} = \sum_{j=1}^{n}(1 + |Hz_j|^2)$ satisfies $\mathbb{E}^{\mu_0}[\tilde{z}] < \infty$.

Then, there exists a constant $c(R)$ such that for all $|Y|, |Y'| < R$

$$d_{\mathsf{Hell}}(\mu, \mu') \le c(R)|Y - Y'|\,.$$

Well-Posedness of the Smoothing Problem

Corollary

Let $Y = (y_1, \ldots, y_N)$ and $Y' = (y'_1, \ldots, y'_N)$ be both contained in a ball of radius R. We denote by μ and μ' the posterior distributions associated with the two data sets Y and Y'. Further, assume that $\tilde{z} = \sum_{j=0}^{N}(1 + |Hz_j|^2)$ satisfies $\mathbb{E}^{\mu_0}[\tilde{z}] < \infty$. Let $f : \mathbb{R}^{N+1 \times n_z} \to \mathbb{R}^p$ be such that $\mathbb{E}_0^{\mu}|f(Z)|^2 < \infty$ with $Z = (z_0, \ldots, z_N)$.

Then, there exists a constant $c(R)$ such that for all $|Y|, |Y'| < R$

$$|\mathbb{E}^{\mu}[f(Z)] - E^{\mu'}[f(Z)]| \leq c(R)|Y - Y'|\,.$$

Filtering Problem

Find the pdf $\mathbb{P}(z_n|y_1, \dots y_n)$ associated with the probability measure on the random variable $z_n|y_1, \dots y_n$, i.e. sequentially update the pdf $\mathbb{P}(z_n|y_1, \dots y_n)$ as n is incremented.

Update $\mathbb{P}(z_{n+1}|y_1, \dots y_{n+1})$ from $\mathbb{P}(z_n|y_1, \dots y_n)$ via

prediction $\quad \mathbb{P}(z_n|y_1, \dots y_n) \mapsto \mathbb{P}(z_{n+1}|y_1, \dots y_n)$ and

analysis $\quad \mathbb{P}(z_{n+1}|y_1, \dots y_n) \mapsto \mathbb{P}(z_{n+1}|y_1, \dots y_{n+1})$.

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- **Prediction**

$$\begin{aligned}\mathbb{P}(z_{n+1}|y_1,\dots y_n) &= \int_{\mathbb{R}^{n_z}} \mathbb{P}(z_{n+1}|y_1,\dots y_n, z_n)\mathbb{P}(z_n|y_1,\dots y_n)\mathrm{d}z_n \\ &= \int_{\mathbb{R}^{n_z}} \mathbb{P}(z_{n+1}|z_n)\mathbb{P}(z_n|y_1,\dots y_n)\mathrm{d}z_n\,.\end{aligned}$$

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- **Analysis**

$$\begin{aligned}\mathbb{P}(z_{n+1}|y_1,\dots y_{n+1}) &= \mathbb{P}(z_{n+1}|y_1,\dots,y_n,y_{n+1})\\ &= \frac{\mathbb{P}(y_{n+1}|z_{n+1},y_1,\dots,y_n)\mathbb{P}(z_{n+1}|y_1,\dots,y_n)}{\mathbb{P}(y_{n+1}|y_1,\dots,y_n)}\\ &= \frac{\mathbb{P}(y_{n+1}|z_{n+1})\mathbb{P}(z_{n+1}|y_1,\dots,y_n)}{\mathbb{P}(y_{n+1}|y_1,\dots,y_n)}.\end{aligned}$$

Relation between Smoothing and Filtering

We denote by $\mathbb{P}(z_0, \ldots, z_N | y_1, \ldots, y_N)$ the smoothing distribution and by $\mathbb{P}(z_N | y_1, \ldots y_N)$ the filtering distribution at time N. Then, the marginal of the smoothing distribution on z_N coincides with the filtering distribution at time N, i.e.

$$\int \mathbb{P}(z_0, \ldots, z_N | y_1, \ldots, y_N) \mathrm{d}z_0 \ldots \mathrm{d}z_{N-1} = \mathbb{P}(z_N | y_1, \ldots y_N) \, .$$

Note that the marginal of the smoothing distribution on $z_n, \ n < N$ is in general **not equal** to the filter $\mathbb{P}(z_n | y_1, \ldots y_n)$.

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Well-Posedness of the Filtering Problem

Corollary

Let $Y = (y_1, \dots, y_N)$ and $Y' = (y'_1, \dots, y'_N)$ be both contained in a ball of radius R. We denote by μ and μ' the smoothing distributions associated with the two data sets Y and Y'. Further, assume that $\tilde{z} = \sum_{j=0}^{N}(1 + |Hz_j|^2)$ satisfies $\mathbb{E}^{\mu_0}[\tilde{z}] < \infty$. Let $g : \mathbb{R}^{n_z} \to \mathbb{R}^p$ be such that $\mathbb{E}^{\mu_0}|g(z_N)|^2 < \infty$.

Then, there exists a constant $c(R)$ such that for all $|Y|, |Y'| < R$

$$|\mathbb{E}^{\mu_N}[g(z_N)] - E^{\mu'}[g(z_N)]| \leq c(R)|Y - Y'|\,,$$

where μ_N and μ'_N denote the filtering distributions at time N corresponding to data z_N and z'_N, i.e. the marginals of μ and μ' in N.

Further Reading

Bayesian Inference

Kaipio and Somersalo 2005, Stuart 2010, Tarantola 2005

Well-posedness

Stuart 2010, Law, Stuart, Zygalakis 2015

Bayesian Estimators

Kaipio and Somersalo 2005, Stuart 2010, Dashti, Law, Stuart and Voss 2013, Agapiou, Burger, Dashti, and Helin 2018

Link to Optimal Transport

Villani 2009, Van Leeuwen, Cheng and Reich 2015, Marzouk, Moselhy, Parno and Spantini 2016

Linear Example

Smoothing Problem

Evolution model

$$z_{n+1} = az_n + \zeta_n \,, \quad j \in \{0, \dots, N\}, \quad z_0 \sim \mathcal{N}(m_0, \sigma^2), \quad \zeta_0 \sim \mathcal{N}(0, \sigma^2)\,.$$

Observation model

$$y_{n+1} = hz_{n+1} + \eta_{n+1} \,, \quad j \in \{1, \dots, N\}, \quad \eta_1 \sim \mathcal{N}(0, \gamma^2)\,.$$

Linear Example

Smoothing Problem

Evolution model

$$z_{n+1} = az_n + \zeta_n\,, \quad j \in \{0, \ldots, N\}, \quad z_0 \sim \mathcal{N}(m_0, \sigma^2), \quad \zeta_0 \sim \mathcal{N}(0, \sigma^2)\,.$$

Observation model

$$y_{n+1} = hz_{n+1} + \eta_{n+1}\,, \quad j \in \{1, \ldots, N\}, \quad \eta_1 \sim \mathcal{N}(0, \gamma^2)\,.$$

Prior

$$P(z_0, \ldots, z_n) \propto \exp(-\Theta(z_0, \ldots, z_n))$$

with

$$\Theta(z_0, \ldots, z_n) = \frac{1}{2\sigma^2}|z_0 - m_0|^2 + \sum_{n=0}^{N-1} \frac{1}{2\sigma^2}|z_{n+1} - az_n|^2\,.$$

Linear Example

Smoothing Problem

Evolution model

$$z_{n+1} = a z_n + \zeta_n\,, \quad j \in \{0,\dots,N\}, \quad z_0 \sim \mathcal{N}(m_0,\sigma^2), \quad \zeta_0 \sim \mathcal{N}(0,\sigma^2)\,.$$

Observation model

$$y_{n+1} = h z_{n+1} + \eta_{n+1}\,, \quad j \in \{1,\dots,N\}, \quad \eta_1 \sim \mathcal{N}(0,\gamma^2)\,.$$

Likelihood

$$\mathbb{P}(y_1,\dots,y_n|z_0,\dots,z_n) \propto \exp(-\Phi(z_0,\dots,z_n;y_1,\dots,y_n)$$

with

$$\Phi(z_0,\dots,z_n;y_1,\dots,y_n) = \sum_{n=0}^{N-1} \frac{1}{2\gamma^2}|y_{n+1} - h z_{n+1}|^2$$

Linear Example

Smoothing Problem

Evolution model

$$z_{n+1} = az_n + \zeta_n\,, \quad j \in \{0,\dots,N\}, \quad z_0 \sim \mathcal{N}(m_0,\sigma^2), \quad \zeta_0 \sim \mathcal{N}(0,\sigma^2)\,.$$

Observation model

$$y_{n+1} = hz_{n+1} + \eta_{n+1}\,, \quad j \in \{1,\dots,N\}, \quad \eta_1 \sim \mathcal{N}(0,\gamma^2)\,.$$

Posterior

$$\mathbb{P}(z_0,\dots,z_n|y_1,\dots,y_n) \propto \exp(-\Phi(z_0,\dots,z_n;y_1,\dots,y_n) - \Theta(z_0,\dots,z_n))\,.$$

Linear Example

Smoothing Problem

Evolution model

$$z_{n+1} = az_n + \zeta_n\,, \quad j \in \{0,\dots,N\}, \quad z_0 \sim \mathcal{N}(m_0,\sigma^2), \quad \zeta_0 \sim \mathcal{N}(0,\sigma^2)\,.$$

Observation model

$$y_{n+1} = hz_{n+1} + \eta_{n+1}\,, \quad j \in \{1,\dots,N\}, \quad \eta_1 \sim \mathcal{N}(0,\gamma^2)\,.$$

Posterior

$$z|y \sim \mathcal{N}(m,C)$$

with

$$C^{-1} = \begin{pmatrix} 1/\sigma^2 + a^2/\sigma^2 & -a/\sigma^2 & & \\ -a/\sigma^2 & h^2/\gamma^2 + a^2/\sigma^2 + 1/\sigma^2 & -a/\sigma^2 & \\ \ddots & \ddots & \ddots & \\ & & & -a/\sigma^2 \\ & & -a/\sigma^2 & h^2/\gamma^2 + 1/\sigma^2 \end{pmatrix},\; C^{-1}m = \begin{pmatrix} m_0/\sigma^2 \\ h/\gamma^2 y_1 \\ \vdots \\ h/\gamma^2 y_n \end{pmatrix}.$$

Linear Example

Filtering Problem

Evolution model

$$z_{n+1} = az_n + \zeta_n \,, \quad j \in \{0, \dots, N\}, \quad z_0 \sim \mathcal{N}(m_0, \sigma^2), \quad \zeta_0 \sim \mathcal{N}(0, \sigma^2) \,.$$

Observation model

$$y_{n+1} = hz_{n+1} + \eta_{n+1} \,, \quad j \in \{1, \dots, N\}, \quad \eta_1 \sim \mathcal{N}(0, \gamma^2) \,.$$

Linear Example

Filtering Problem

Evolution model

$$z_{n+1} = az_n + \zeta_n\,, \quad j \in \{0,\dots,N\}, \quad z_0 \sim \mathcal{N}(m_0,\sigma^2), \quad \zeta_0 \sim \mathcal{N}(0,\sigma^2)\,.$$

Observation model

$$y_{n+1} = hz_{n+1} + \eta_{n+1}\,, \quad j \in \{1,\dots,N\}, \quad \eta_1 \sim \mathcal{N}(0,\gamma^2)\,.$$

Prediction

$$\begin{aligned}
\mathbb{P}(z_{n+1}|y_1,\dots y_n) &= \int_{\mathbb{R}^{n_z}} \mathbb{P}(z_{n+1}|y_1,\dots y_n, z_n)\mathbb{P}(z_n|y_1,\dots y_n)\mathrm{d}z_n \\
&= \int_{\mathbb{R}^{n_z}} \mathbb{P}(z_{n+1}|z_n)\mathbb{P}(z_n|y_1,\dots y_n)\mathrm{d}z_n\,.
\end{aligned}$$

Linear Example

Filtering Problem

Evolution model

$$z_{n+1} = az_n + \zeta_n\,, \quad j \in \{0,\dots,N\}, \quad z_0 \sim \mathcal{N}(m_0,\sigma^2), \quad \zeta_0 \sim \mathcal{N}(0,\sigma^2)\,.$$

Observation model

$$y_{n+1} = hz_{n+1} + \eta_{n+1}\,, \quad j \in \{1,\dots,N\}, \quad \eta_1 \sim \mathcal{N}(0,\gamma^2)\,.$$

Prediction

$$z_{n+1}|y_1,\dots y_n \sim \mathcal{N}(am_n, a^2c_n+\sigma^2) = \mathcal{N}(\hat{m}_{n+1},\hat{c}_{n+1})$$

with

$$z_n|y_1,\dots y_n \sim \mathcal{N}(m_n,c_n)$$

Linear Example

Filtering Problem

Evolution model

$$z_{n+1} = az_n + \zeta_n\,, \quad j \in \{0,\ldots,N\}, \quad z_0 \sim \mathcal{N}(m_0,\sigma^2), \quad \zeta_0 \sim \mathcal{N}(0,\sigma^2)\,.$$

Observation model

$$y_{n+1} = hz_{n+1} + \eta_{n+1}\,, \quad j \in \{1,\ldots,N\}, \quad \eta_1 \sim \mathcal{N}(0,\gamma^2)\,.$$

Analysis

$$\mathbb{P}(z_{n+1}|y_1,\ldots y_{n+1}) \quad = \quad \frac{\mathbb{P}(y_{n+1}|z_{n+1})\mathbb{P}(z_{n+1}|y_1,\ldots,y_n)}{\mathbb{P}(y_{n+1}|y_1,\ldots,y_n)}\,.$$

Linear Example

Filtering Problem

Evolution model

$$z_{n+1} = az_n + \zeta_n\,, \quad j \in \{0, \dots, N\}, \quad z_0 \sim \mathcal{N}(m_0, \sigma^2), \quad \zeta_0 \sim \mathcal{N}(0, \sigma^2)\,.$$

Observation model

$$y_{n+1} = hz_{n+1} + \eta_{n+1}\,, \quad j \in \{1, \dots, N\}, \quad \eta_1 \sim \mathcal{N}(0, \gamma^2)\,.$$

Analysis

$$z_{n+1}|y_1, \dots y_{n+1} \sim \mathcal{N}(m_{n+1}, c_{n+1})$$

with

$$\begin{aligned} m_{n+1} &= \hat{m}_{n+1} + \hat{c}_{n+1} h (h \hat{c}_{n+1} h + \gamma^2)^{-1} (y_{n+1} - h\hat{m}_{n+1}) \\ c_{n+1} &= \hat{c}_{n+1} - \hat{c}_{n+1} h (h \hat{c}_{n+1} h + \gamma^2)^{-1} h \hat{c}_{n+1} \\ z_{n+1}|y_1, \dots y_n &\sim \mathcal{N}(\hat{m}_{n+1}, \hat{c}_{n+1})\,. \end{aligned}$$

Linear Example

Evolution model

$$z_{n+1} = 1.2 z_n + \zeta_n\,, \quad j \in \{0, \dots, 10\}, \quad z_0 \sim \mathcal{N}(1, 0.01), \quad \zeta_0 \sim \mathcal{N}(0, 0.01)\,.$$

Observation model

$$y_{n+1} = 1 z_{n+1} + \eta_{n+1}\,, \quad j \in \{1, \dots, 10\}, \quad \eta_1 \sim \mathcal{N}(0, 0.1)\,.$$

Linear Example

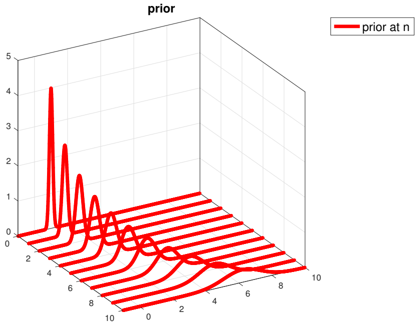
Evolution model

$$z_{n+1} = 1.2 z_n + \zeta_n\,, \quad j \in \{0,\dots,10\}, \quad z_0 \sim \mathcal{N}(1, 0.01), \quad \zeta_0 \sim \mathcal{N}(0, 0.01)\,.$$

Observation model

$$y_{n+1} = 1 z_{n+1} + \eta_{n+1}\,, \quad j \in \{1,\dots,10\}, \quad \eta_1 \sim \mathcal{N}(0, 0.1)\,.$$

Smoothing



Linear Example

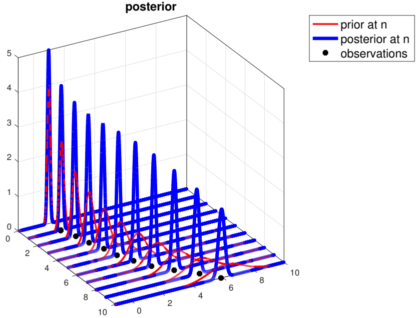
Evolution model

$$z_{n+1} = 1.2 z_n + \zeta_n\,, \quad j \in \{0, \dots, 10\}, \quad z_0 \sim \mathcal{N}(1, 0.01), \quad \zeta_0 \sim \mathcal{N}(0, 0.01)\,.$$

Observation model

$$y_{n+1} = 1 z_{n+1} + \eta_{n+1}\,, \quad j \in \{1, \dots, 10\}, \quad \eta_1 \sim \mathcal{N}(0, 0.1)\,.$$

Smoothing



Linear Example

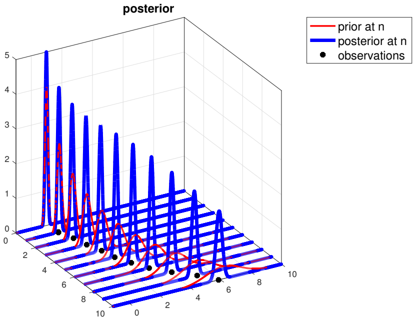
Evolution model

$$z_{n+1} = 1.2 z_n + \zeta_n\,, \quad j \in \{0, \dots, 10\}, \quad z_0 \sim \mathcal{N}(1, 0.01), \quad \zeta_0 \sim \mathcal{N}(0, 0.01)\,.$$

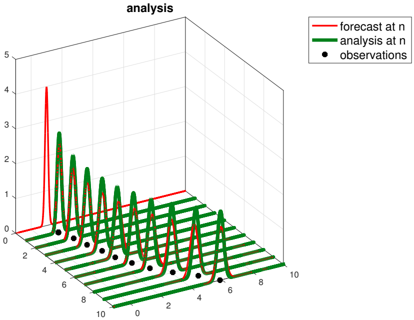
Observation model

$$y_{n+1} = 1 z_{n+1} + \eta_{n+1}\,, \quad j \in \{1, \dots, 10\}, \quad \eta_1 \sim \mathcal{N}(0, 0.1)\,.$$

Smoothing



Filtering



Linear Example

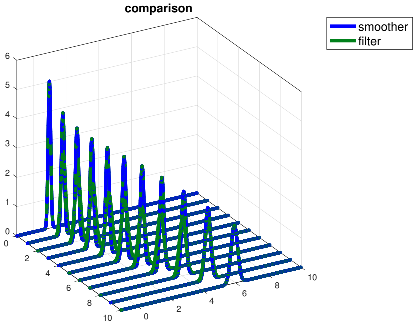
Evolution model

$$z_{n+1} = 1.2 z_n + \zeta_n\,, \quad j \in \{0, \ldots, 10\}, \quad z_0 \sim \mathcal{N}(1, 0.01), \quad \zeta_0 \sim \mathcal{N}(0, 0.01)\,.$$

Observation model

$$y_{n+1} = 1 z_{n+1} + \eta_{n+1}\,, \quad j \in \{1, \ldots, 10\}, \quad \eta_1 \sim \mathcal{N}(0, 0.1)\,.$$

Comparison Smoothing and Filtering



Kalman Smoother

For a **linear model** $z_{n+1} = Az_n + \zeta_n$ with $A \in \mathcal{L}(\mathbb{R}^{n_z}, \mathbb{R}^{n_z})$ and **linear observations** $y_{n+1} = Hz_{n+1} + \eta_{n+1}$ with $H \in \mathcal{L}(\mathbb{R}^{n_z}, \mathbb{R}^{n_y})$, the conditional density $\mathbb{P}(Z|Y)$ is proportional to

$$\exp(-\frac{1}{2}\sum_{j=0}^{N-1}|y_{j+1} - Hz_{j+1}|_{\Gamma}^2 - \frac{1}{2}\sum_{j=0}^{N-1}|z_{j+1} - Az_j|_{\Sigma}^2 - \frac{1}{2}|z_0 - m_0|_{C_0}^2)\,.$$

Kalman Smoother

Kalman Smoother

The posterior smoothing distribution on $Z|Y$ for the linear dynamics model is a Gaussian measure $\mu = \mathcal{N}(m, C)$ on $\mathbb{R}^{N+1\times n_z}$.

The covariance C is the inverse of a symmetric positive definite precision matrix

$$L = \begin{pmatrix} L_{11} & L_{12} & & & \\ L_{21} & L_{22} & L_{23} & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & L_{NN+1} \\ & & & L_{N+1N} & L_{N+1N+1} \end{pmatrix}$$

with $L_{ij} \in \mathbb{R}^{n_z \times n_z}$, $L_{11} = C_0^{-1} + A^\top \Sigma^{-1} A$, $L_{jj} = H^\top \Gamma^{-1} H + A^\top \Sigma^{-1} A + \Sigma^{-1}$ for $j = 2, \ldots, N$, $L_{N+1N+1} = H^\top \Gamma^{-1} H + \Sigma^{-1}$, $L_{jj+1} = -A^\top \Sigma^{-1}$, $L_{jj+1} = -\Sigma^{-1} A$ for $j = 1, \ldots, N$.

The mean m solves

$$Lm = r$$

with $r_1 = C_0^{-1} m_0$, $r_j = H^\top \Gamma^{-1} y_{j-1}$ for $j = 2, \ldots, J+1$.

Kalman Smoother

The mean of the posterior smoothing distribution $\mu = \mathcal{N}(m, C)$ is a minimizer of the functional

$$J(Z,Y) = -\frac{1}{2}\sum_{j=0}^{N-1} |y_{j+1} - Hz_{j+1}|_{\Gamma}^2 + \frac{1}{2}\sum_{j=0}^{N+1} |z_{j+1} - Az_j|_{\Sigma}^2 - \frac{1}{2}|z_0 - m_0|_{C_0}^2$$

w.r. to Z.

The inverse covariance is given by the Hessian matrix of the functional J.

Kalman Filter

For a **linear model** $z_{n+1} = Az_n + \zeta_n$ with $A \in \mathcal{L}(\mathbb{R}^{n_z}, \mathbb{R}^{n_z})$ and **linear observations** $y_{n+1} = Hz_{n+1} + \eta_{n+1}$ with $H \in \mathcal{L}(\mathbb{R}^{n_z}, \mathbb{R}^{n_y})$, the filtering problem is to estimate the state at time j given the data from the past up to time j, i.e. the goal of computation is the pdf associated with the measure on the random variable $z_j|y_1, \dots y_j$.

We consider

Prediction Step $\hat{\mu}_{j+1} = \mathcal{P}\mu_j$

Analysis Step $\mu_{j+1} = \mathcal{L}_j \hat{\mu}_{j+1}$.

Then, the prediction and analysis step provide a mapping from

$$\mathbb{P}(z_j|y_1, \dots y_j)$$

to

$$\mathbb{P}(z_{j+1}|y_1, \dots y_{j+1}).$$

Kalman Filter

Kalman Filter

The filtering distribution on $z_j|y_1, \dots y_j$ for the linear dynamics model is a Gaussian measure $\mu_j = \mathcal{N}(m_j, C_j)$ on $\mathbb{R}^{n_z}$.

The covariance C_j is symmetric positive definite and the inverse is given by

$$C_{j+1}^{-1} = (AC_jA^\top + \Sigma)^{-1} + H^\top \Gamma^{-1} H$$

and the mean is determined by

$$C_{j+1}^{-1} m_{j+1} = (AC_jA^\top + \Sigma)^{-1} Am_j + H^\top \Gamma^{-1} y_{j+1}\,.$$

Kalman Filter

For a **linear model** $z_{n+1} = Az_n + \zeta_n$ with $A \in \mathcal{L}(\mathbb{R}^{n_z}, \mathbb{R}^{n_z})$ and **linear observations** $y_{n+1} = Hz_{n+1} + \eta_{n+1}$ with $H \in \mathcal{L}(\mathbb{R}^{n_z}, \mathbb{R}^{n_y})$, the conditional density $\mathbb{P}(z_{n+1}|y_1, \ldots y_{n+1})$ is proportional to

$$\exp(-\frac{1}{2}|y_{n+1} - Hz_{n+1}|_\Gamma^2 - \frac{1}{2}|z_{n+1} - \hat{m}_{n+1}|_{\hat{C}_{n+1}}^2)$$

where $(\hat{m}_{n+1}, \hat{C}_{n+1}) = (Am_n, AC_nA^\top + \Sigma)$ is the **forecast mean and covariance**.

We have $z_{n+1}|y_1, \ldots y_{n+1} \sim \mathcal{N}(m_{n+1}, C_{n+1})$ with

$$\begin{aligned} m_{n+1} &= (I - K_{n+1}H)\hat{m}_{n+1} + K_{n+1}y_{n+1} \\ C_{n+1} &= (I - K_{n+1}H)\hat{C}_{n+1} \end{aligned}$$

where $K_{n+1} = \hat{C}_{n+1}H^\top(\Gamma + H\hat{C}_{n+1}H^\top)^{-1}$ is the **Kalman gain**.

Kalman Filter

- The filter is named after Rudolf E. Kálmán.

  R. Kalman and R. Bucy **1961** ***A new approach to linear filtering and prediction problems*** *Journal of Basic Engineering* **82**

- Widely used in practice for control tasks, time series analysis, trajectory optimization, ...

- Gaussian linear assumption.

- Connection to deterministic optimization approaches ($\rightarrow$ 3DVAR, 4DVAR).

- Extensions to nonlinear systems with non Gaussian prior distributions, $\rightarrow$ Ensemble Kalman filter.

  G. Evensen **2003** ***The ensemble Kalman filter: Theoretical formulation and practical implementation*** *Ocean dynamics* **53**

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